



Yasuda-Shedlovsky Result

Sample name: **CS000256**
Assay name: **Fast UV psKa**
Assay ID: **11H-31015**
Filename: **E:\T3 DATA\1108\11H-31015_CS000256_Fast UV psKa.t3r**

Experiment start time: **31/08/2011 19:59:21**
Analyst:
Instrument ID: **T311042**

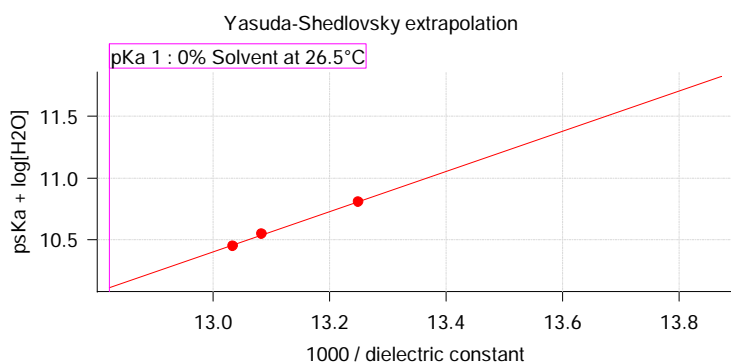
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	8.37	±0.03	-10.71	1623.9800	0.9972	0.212 M	26.5°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11H-31015 Points 104 to 154	23.11 %	Up	UV-metric pKa	76.7	43.4 M	0.215 M	26.8°C	✓ 8.81
11H-31015 Points 53 to 103	31.05 %	Up	UV-metric pKa	76.4	39.2 M	0.215 M	26.3°C	✓ 8.96
11H-31015 Points 3 to 52	40.67 %	Up	UV-metric pKa	75.5	34.1 M	0.206 M	26.5°C	✓ 9.27

Graphs

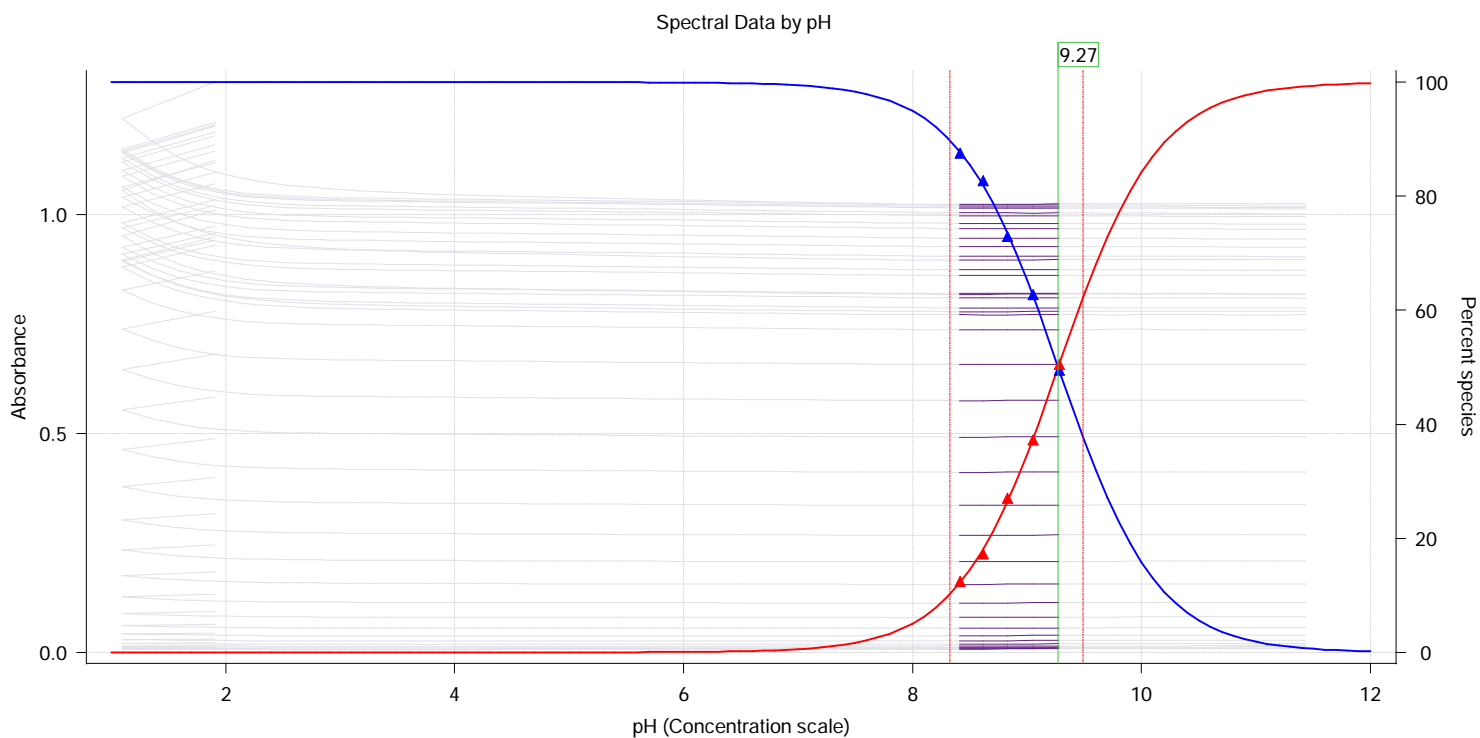
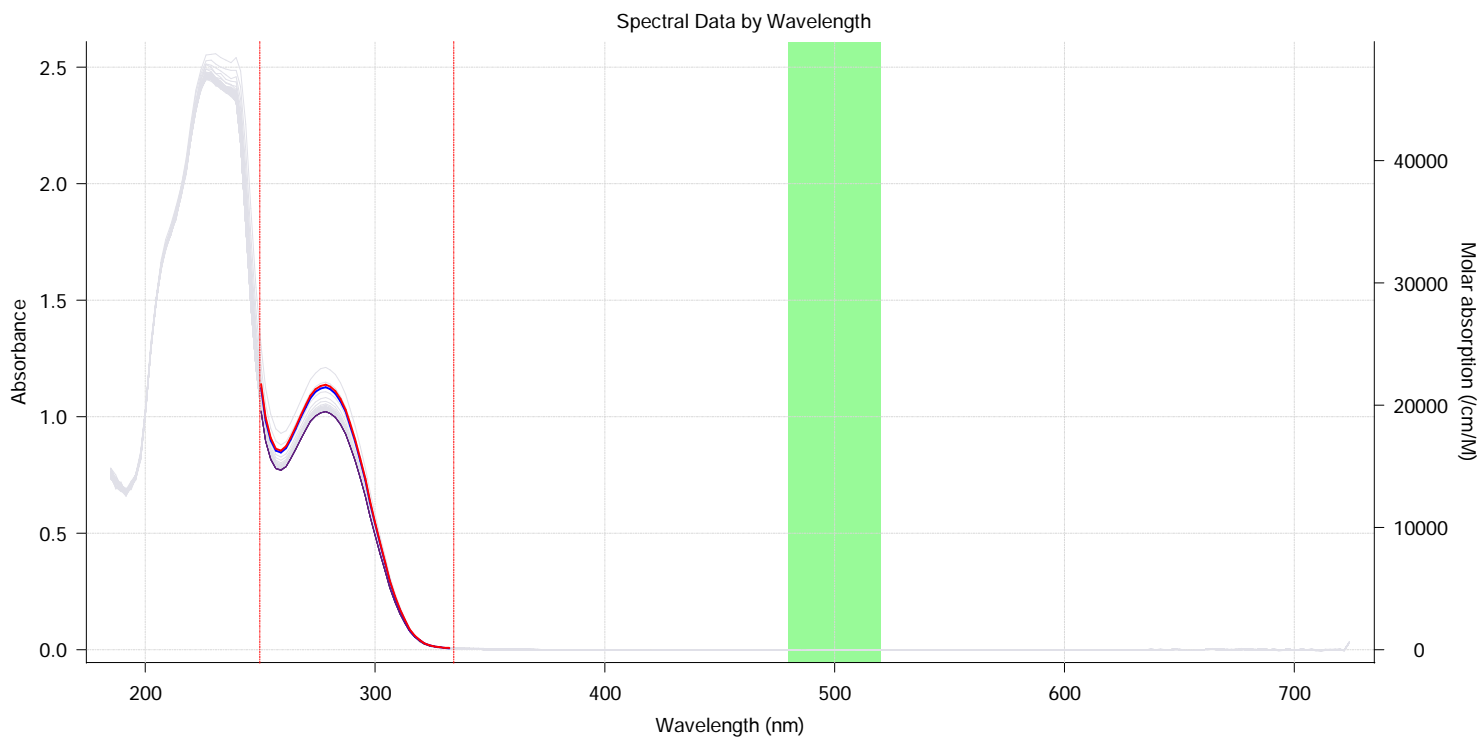


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Fast UV psKa Titration 1 of 3 11H-31015 Points 3 to 52

Graphs

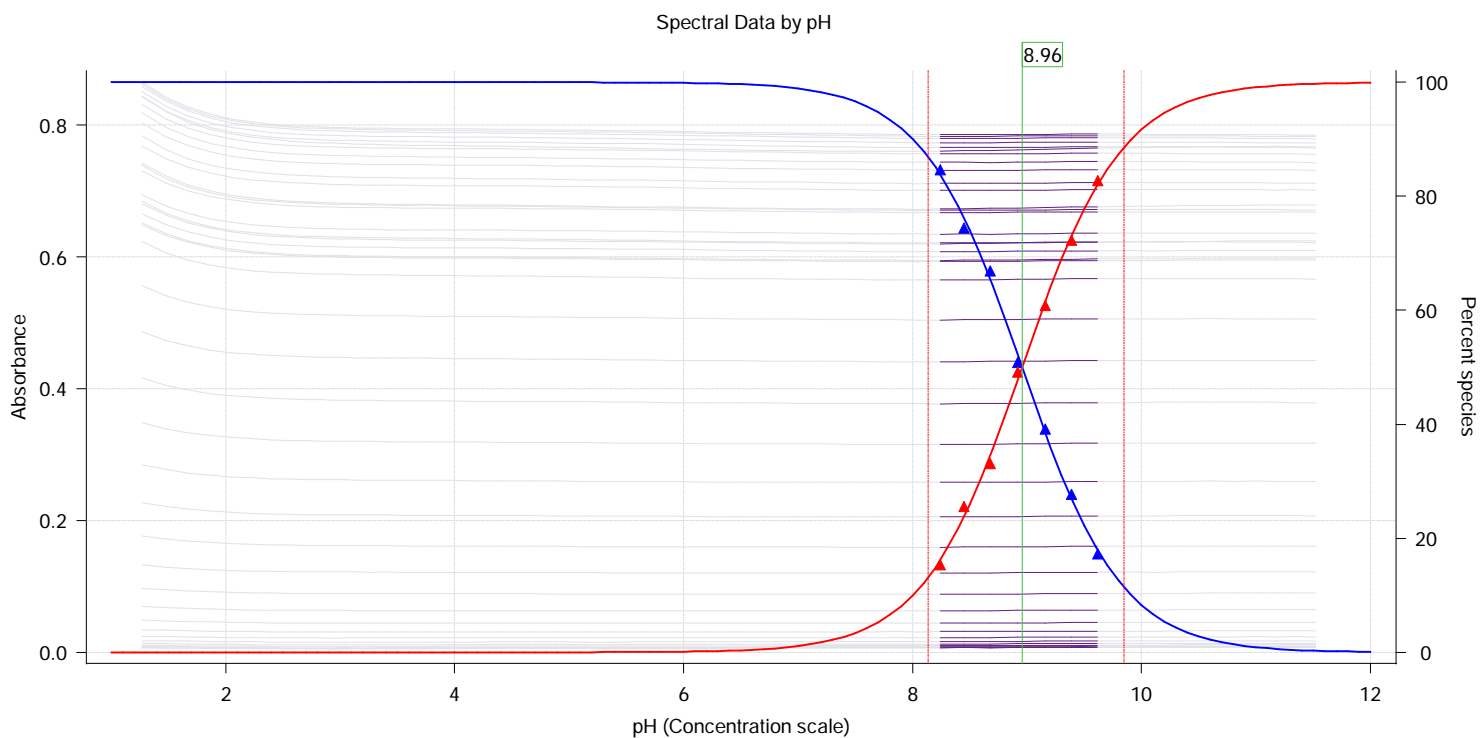
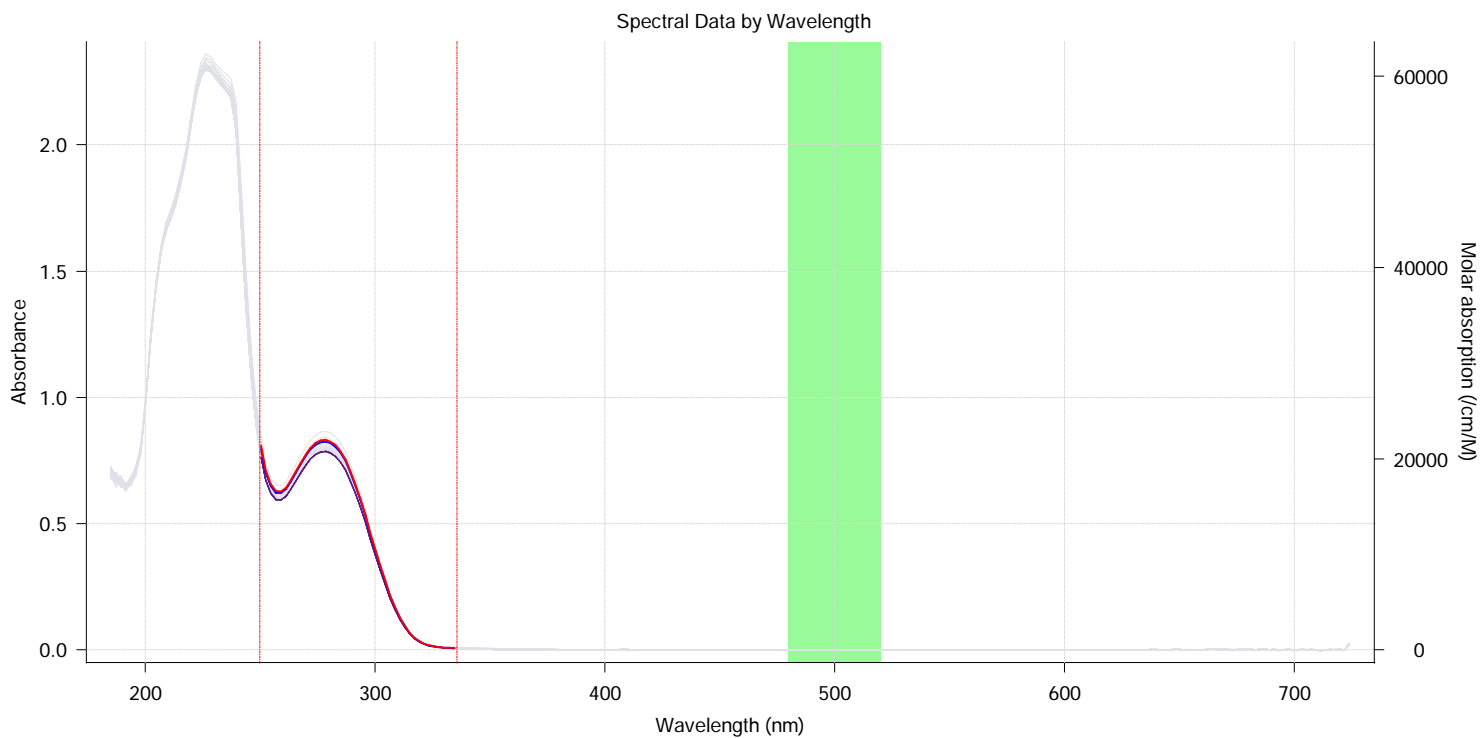


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Fast UV psKa Titration 2 of 3 11H-31015 Points 53 to 103

Graphs

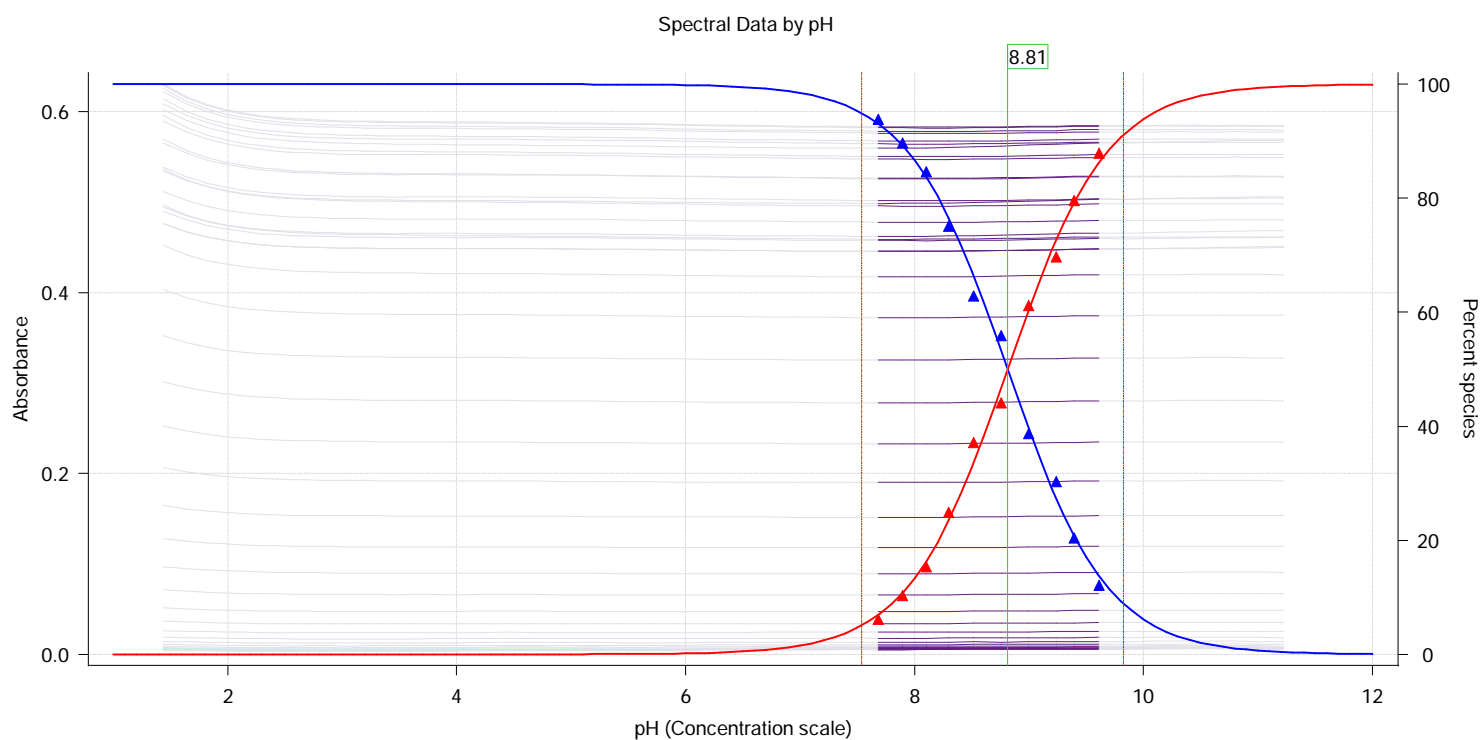
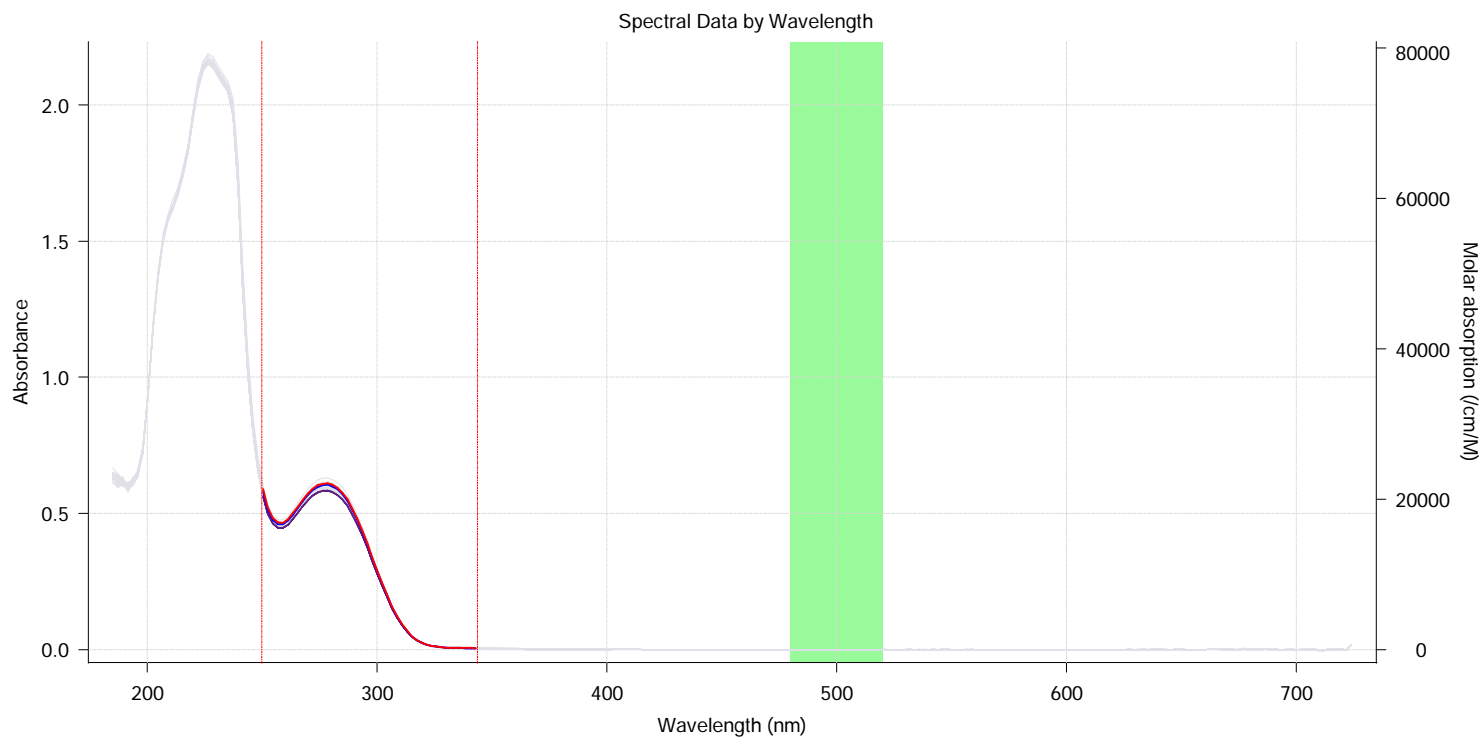


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Fast UV psKa Titration 3 of 3 11H-31015 Points 104 to 154

Graphs





Assay model

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Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000256		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown		
Molecular weight	503.35		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	8.30		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		
